Acetamide, 2,2-dichloro-n-[beta-hydroxy-alpha-(hydroxymeth threo-

InChi:	InChI=1S/C12H12Cl2F3NO5S/c13-10(14)11(21)18-8(5-19)9(20)6-1-3-7(4-2-6)24(22,23)1
InchiKey:	AOZYFDLPICIRLC-UHFFFAOYSA-N
Formula:	C12H12Cl2F3NO5S
SMILES:	O=C(NC(CO)C(O)c1ccc(S(=O)(=O)C(F)(F)F)cc1)C(Cl)Cl
Mol. weight [g/mol]:	410.19
CAS:	309-18-2

Physical Properties

Property code	Value	Unit	Source
gf	-1241.54	kJ/mol	Joback Method
hf	-1527.27	kJ/mol	Joback Method
hfus	46.39	kJ/mol	Joback Method
hvap	114.28	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	1.294		Crippen Method
mcvol	237.350	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
tb	909.92	K	Joback Method
tc	1115.75	K	Joback Method
tf	545.76	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.68	J/mol×K	909.92	Joback Method
cpg	680.59	J/mol×K	944.22	Joback Method
cpg	686.72	J/mol×K	978.53	Joback Method
cpg	692.10	J/mol×K	1012.83	Joback Method
cpg	696.78	J/mol×K	1047.14	Joback Method
cpg	700.82	J/mol×K	1081.44	Joback Method
cpg	704.25	J/mol×K	1115.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C309182&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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